AUTHOR INDEX TO VOLUME 112

Ames, D.E., see M.H. Palmer 112 (1987) 213
Andrews, D.L., A new magneto-optical effect in Raman spectroscopy 112 (1987) 61
Anikin, S.A., see V.A. Avetisov 112 (1987) 179
Anisimov, O.A., see V.V. Lozovoy 112 (1987) 463
Avetisov, V.A., V.V. Kuz'min and S.A. Anikin, Sensitivity of chemical chiral systems to weak asymmetric factors 112 (1987) 179

Bak, T.A. and B. Lu, The general solution of the coagulation equation for branched polymers 112 (1987) 189
Barbeschi, M., L. Bencivenni and F. Ramondo, IR matrix spectra of $CsNO_2$, $RbNO_2$, KNO_2 and $NaNO_2$. The structure of $CsNO_2$ 112 (1987) 387
Bässler, H., see A. Elschner 112 (1987) 285
Benassi, P., see V. Mazzacurati 112 (1987) 147
Bencivenni, L., see M. Barbeschi 112 (1987) 387
Bilkis, I.I., see V.V. Lozovoy 112 (1987) 463
Billing, G.D., Cross sections for rotational/vibrational transitions in HF–HF collisions: effect of initial state 112 (1987) 95
Blake, A.J., see M.H. Palmer 112 (1987) 213
Blomquist, J. and H. Essén, Correlation and the charge distribution of atoms 112 (1987) 173
Breitenstein, M., H. Meyer and A. Schweig, CI calculations of electron and X-ray scattering cross sections of non-linear molecules: H_2O and NH_3 112 (1987) 199
Brickman, R.O., see M.R. Levy 112 (1987) 123
Buckingham, A.D., P.W. Fowler and P.A. Galwas, Velocity-dependent property surfaces and the theory of vibrational circular dichroism 112 (1987) 1
Buemi, G., see A. Raudino 112 (1987) 77
Buenker, R.J., see G. Theodorakopoulos 112 (1987) 319
Büsener, H., F. Heinrich and A. Hese, Electric dipole moments of the MgO $B\,^1\Sigma^+$ and $X\,^1\Sigma^+$ states 112 (1987) 139

Clary, D.C. and S. Green, Test of a modified sudden approximation for rotational excitation in He + CH_3CN 112 (1987) 15
Cooper, I.L., Perturbational and variational treatments of the Morse oscillator 112 (1987) 67
Cox, D.M., see M.R. Levy 112 (1987) 105
Cramarossa, F., see S. de Benedictis 112 (1987) 363

Davidsson, Å., see L.B.-Å. Johansson 112 (1987) 373
De Benedictis, S. and F. Cramarossa, Vibrational analysis of $N_2(B\,^3\Pi_g$ and $C\,^3\Pi_u)$ and CO(X) excited in N_2 discharge and post discharge 112 (1987) 363
De Vivie, R., C.M. Marian and S.D. Peyerimhoff, Spin-forbidden transitions in the presence of an intersystem crossing: application to the $b\,^1\Sigma^+$ state in OH^+ 112 (1987) 349
Decleva, P. and A. Lisini, Calculation of the valence shell correlation effects on ionization potentials. A test on N_2, C_2N_2 and H_2NN 112 (1987) 339

Diercksen, G.H.F. and P.W. Langhoff, Theoretical studies of photoexcitation and ionization in hydrogen sulfide 112 (1987) 227

Elschner, A. and H. Bässler, Site-selective fluorescence and hole-burning spectroscopy of MTHF glasses doped wih tetracene or pentacene 112 (1987) 285
Essén, H., see J. Blomquist 112 (1987) 173

Fantoni, R., K. van Helvoort, W. Knippers and J. Reuss, Direct observation of torsional levels in Raman spectra of C_2H_6. Chem. Phys. 110 (1986) 1. Erratum 112 (1987) 472
Ferguson, J. and E. Krausz, Magnetically perturbed, temperature-dependent and time-resolved aspects of the polarized luminescence of $Ru(bpy)_3^{2+}$ below 10 K 112 (1987) 271
Fleming, J.W., see S. Zabarnick 112 (1987) 409
Fowler, P.W., see A.D. Buckingham 112 (1987) 1

Galimov, R.R., see A.V. Yurkovskaya 112 (1987) 259
Galwas, P.A., see A.D. Buckingham 112 (1987) 1
Goscinski, O., see V. Mujica 112 (1987) 159
Gould, R.O., see M.H. Palmer 112 (1987) 213
Green, S., see D.C. Clary 112 (1987) 15
Grigoryants, V.M., see V.V. Lozovoy 112 (1987) 463

Heinrich, F., see H. Büsener 112 (1987) 139
Hese, A., see H. Büsener 112 (1987) 139

Iskanderov, T.A., Ya.M. Kimel'fel'd and E.M. Smirnova, Infrared spectroscopic studies of hydrogen-bonded complexes in cryogenic solutions 112 (1987) 379

Johansson, L.B.-Å., G. Wikander, G. Lindblom and Å. Davidsson, Linear dichroism of molecules with cubic symmetry 112 (1987) 373

Kaldor, A., see M.R. Levy 112 (1987) 105
Kaldor, A., see M.R. Levy 112 (1987) 123
Karabunarliev, S.H., see N.N. Tyutyulkov 112 (1987) 293
Kimel'fel'd, Ya.M., see T.A. Iskanderov 112 (1987) 379
Klein, J., see P. Petelenz 112 (1987) 457
Knippers, W., see R. Fantoni 112 (1987) 472
Krausz, E., see J. Ferguson 112 (1987) 271
Kuz'min, V.V., see V.A. Avetisov 112 (1987) 179

Langen, J., K.-P. Lodemann and U. Schurath, Effect of guest–host interaction on spectra and relaxation dynamics of matrix-isolated Br_2 $B^3\Pi_{0^+u}$, $A^3\Pi_{1u}$ and $A'^3\Pi_{2u}$ 112 (1987) 393
Langhoff, P.W., see G.H.F. Diercksen 112 (1987) 227
Larter, R. and D.J. Malik, Effects of non-uniform electric fields on the convergence behavior of energy expansions 112 (1987) 301
Lazzeretti, P., see J.A. Tossel 112 (1987) 205
Lee, D.H. and R.E.D. McClung, The Fokker–Planck–Langevin model for rotational brownian motion. IV. Asymmetric top molecules 112 (1987) 23
Levy, M.R., D.M. Cox and A. Kaldor, IR laser-induced decomposition of volatile uranyl complexes. I. Analysis of molecular beam depletions 112 (1987) 105

Levy, M.R., R.O. Brickman and A. Kaldor, IR laser-induced decomposition of volatile uranyl complexes. II. New double resonance results 112 (1987) 123
Li, Y., see V. Mujica 112 (1987) 159
Lin, M.C., see S. Zabarnick 112 (1987) 409
Lindblom, G., see L.B.-Å. Johansson 112 (1987) 373
Lisini, A., see P. Decleva 112 (1987) 339
Lodemann, K.-P., see J. Langen 112 (1987) 393
Loesch, H., The effect of reagent rotation on reaction cross sections for $O(^3P) + HCl \rightarrow OH + Cl$: a rationale for contradictory predictions 112 (1987) 85
Lőrincz, A., Possibility of detecting oscillations in near resonance Raman scattering 112 (1987) 245
Lozovoy, V.V., V.M. Grigoryants, O.A. Anisimov, Yu.N. Molin, P.V. Schastnev, L.N. Shchegoleva, I.I. Bilkis and V.D. Shteingarts, The hfi parameters and structure of radical-anions of substituted tetra- and pentafluorobenzenes. Theory and experiment (OD ESR) 112 (1987) 463
Lu, B., see T.A. Bak 112 (1987) 189

Madden, P.A. and F. van Swol, Comparison of the rate constants for VV energy transfer in the gas and liquid phases 112 (1987) 43
Malik, D.J., see R. Larter 112 (1987) 301
Mangle, E.A. and M.R. Topp, Jet spectroscopy of pyrene complexes: unusual complexation shifts in the $S_0 \rightarrow S_1$ spectrum 112 (1987) 427
Mangle, E.A., A.L. Motyka, P. Salvi and M.R. Topp, The effect of molecular symmetry in alkane complexes of 2,5-diphenylfuran and related species 112 (1987) 443
Marian, C.M., see R. de Vivie 112 (1987) 349
Martin, P., see P. Petelenz 112 (1987) 457
Mazzacurati, V. and P. Benassi, Fabry–Perot spectra of depolarized Rayleigh wing in water: a new analysis of its temperature dependence 112 (1987) 147
McClung, R.E.D., see D.H. Lee 112 (1987) 23
Meyer, H., see M. Breitenstein 112 (1987) 199
Molin, Yu.N., see V.V. Lozovoy 112 (1987) 463
Motyka, A.L., see E.A. Mangle 112 (1987) 443
Mujica, V., Y. Li and O. Goscinski, Dynamic coordinate separation and state-dependent potentials. An analysis of localization in helium 112 (1987) 159

Nicolaides, C.A., see G. Theodorakopoulos 112 (1987) 319
Nishimura, Y., see N. Nishiyama 112 (1987) 265
Nishiyama, N., H. Sekiya, M. Tsuji and Y. Nishimura, Internal energy disposal in the chemiluminescent reaction CD + NO → ND(A) + CO and the kinetic isotope effect 112 (1987) 265

Obynochny, A.A., see A.V. Yurkovskaya 112 (1987) 259

Palmer, M.H., R.O. Gould, A.J. Blake, J.A.S. Smith, D. Stephenson and D.E. Ames, ^{14}N nuclear quadrupole coupling in solid cinnolin-4-ones. A study by nuclear quadrupole resonance, X-ray crystallography and ab initio calculations 112 (1987) 213
Panas, I., P. Siegbahn and U. Wahlgren, Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. I. The design of a one-electron effective core potential which includes 3d relaxation effects 112 (1987) 325

Petelenz, P., V.H. Smith Jr., J. Klein, P. Martin and R. Voltz, Recombination of charge carriers in anthracene 112 (1987) 457
Petsalakis, I.D., see G. Theodorakopoulos 112 (1987) 319
Peyerimhoff, S.D., see R. de Vivie 112 (1987) 349
Popa, V.T., see M.O. Vlad 112 (1987) 307

Ramondo, F., see M. Barbeschi 112 (1987) 387
Raudino, A., F. Zuccarello and G. Buemi, Electrostatic solvation energy in electrolyte solutions: a self-consistent inhomogeneous continuum model 112 (1987) 77
Reuss, J., see R. Fantoni 112 (1987) 472
Ross, U. and T. Schulze, Charge-transfer collisions of potassium and rubidium with chlorine clusters: collision-energy dependence of cluster-products 112 (1987) 415

Sagdeev, R.Z., see A.V. Yurkovskaya 112 (1987) 259
Salikhov, K.M., see A.V. Yurkovskaya 112 (1987) 259
Salvi, P., see E.A. Mangle 112 (1987) 443
Schastnev, P.V., see V.V. Lozovoy 112 (1987) 463
Schulze, T., see U. Ross 112 (1987) 415
Schurath, U., see J. Langen 112 (1987) 393
Schweig, A., see M. Breitenstein 112 (1987) 199
Sekiya, H., see N. Nishiyama 112 (1987) 265
Serebrennikov, Yu.A., Zero-field NMR and NQR line shapes in the presence of brownian rotational reorientations 112 (1987) 253
Shchegoleva, L.N., see V.V. Lozovoy 112 (1987) 463
Shteingarts, V.D., see V.V. Lozovoy 112 (1987) 463
Siegbahn, P., see I. Panas 112 (1987) 325
Smirnova, E.M., see T.A. Iskanderov 112 (1987) 379
Smith, J.A.S., see M.H. Palmer 112 (1987) 213
Smith Jr., V.H., see P. Petelenz 112 (1987) 457
Stephenson, D., see M.H. Palmer 112 (1987) 213

Theodorakopoulos, G., I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker, Non-orthonormal basis calculations of the dipole transition moment for the Phillips system ($A^1\Pi_u \rightarrow X^1\Sigma_g^+$) in C_2. Theoretical lifetime of the $A^1\Pi_u$ state 112 (1987) 319
Topp, M.R., see E.A. Mangle 112 (1987) 427
Topp, M.R., see E.A. Mangle 112 (1987) 443
Tossel, J.A. and P. Lazzeretti, Ab initio calculations of oxygen nuclear quadrupole coupling constants and oxygen and silicon NMR shielding constants in molecules containing Si–O bonds 112 (1987) 205
Tsuji, M., see N. Nishiyama 112 (1987) 265
Tyutyulkov, N.N. and S.H. Karabunarliev, Structure and properties of non-classical polymers. IV. Magnetic properties of polymers with superexchange interaction 112 (1987) 293

Van Helvoort, K., see R. Fantoni 112 (1987) 472
Van Swol, F., see P.A. Madden 112 (1987) 43
Vlad, M.O. and V.T. Popa, Age distributions in chemical kinetics 112 (1987) 307
Voltz, R., see P. Petelenz 112 (1987) 457

Wahlgren, U., see I. Panas 112 (1987) 325
Wikander, G., see L.B.-Å. Johansson 112 (1987) 373

Yurkovskaya, A.V., R.R. Galimov, A.A. Obynochny, K.M. Salikhov and R.Z. Sagdeev, The field dependence of CIDNP in gas-phase reactions of biradicals 112 (1987) 259

Zabarnick, S., J.W. Fleming and M.C. Lin, Kinetics of CH($X\,^2\Pi$) radical reactions with propane, isobutane and neopentane 112 (1987) 409
Zuccarello, F., see A. Raudino 112 (1987) 77
Zusman, L.D., Outer-sphere electron transfer reactions at an electrode 112 (1987) 53

0301-0104/87/$03.50 © Elsevier Science Publishers B.V.
(North-Holland Physics Division)

LIST OF SUBJECTS

1 METHODS

1.1 Theoretical

1.1.1 Group theory and algebras
1.1.2 Classical mechanics *
1.1.3 Quantized field theory
1.1.4 Many body and quasiparticle approaches
1.1.5 Coupling schemes and perturbative treatments
1.1.6 Relativistic quantum mechanics *
1.1.7 Transport quantum mechanics *
1.1.8 Equilibrium statistical mechanics
1.1.9 Statistical mechanics of stationary states
1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories
1.1.11 Ab initio schemes for stationary properties
1.1.12 Computational and simulation methods
1.1.13 Molecular dynamics and scattering theory

1.2 Experimental

1.2.1 Magnetic resonances
1.2.2 Cyclotron resonance *
1.2.3 Microwave spectroscopy *
1.2.4 Infrared spectroscopy
1.2.5 Raman spectroscopy
1.2.6 Visible and UV spectroscopy
1.2.7 Fluorescence spectroscopy
1.2.8 Photoelectron and Auger spectroscopy *
1.2.9 X-ray spectroscopy *
1.2.10 Electron impact spectroscopy *
1.2.11 Laser methods
1.2.12 Picosecond spectroscopy *
1.2.13 Non-linear optical spectroscopy *
1.2.14 Synchrotron spectroscopies *
1.2.15 Coherent optical spectroscopy *
1.2.16 Optical pumping *
1.2.17 Multiple resonance spectroscopy
1.2.18 Optoacoustic spectroscopy *
1.2.19 Atomic and molecular beam techniques
1.2.20 Time-resolved experiments
1.2.21 Mass spectrometry *
1.2.22 Radiolysis *
1.2.23 Mössbauer spectroscopy *
1.2.24 X-ray, electron and neutron diffraction
1.2.25 Neutron scattering *
1.2.26 Light scattering
1.2.27 Field emission and field ionization *
1.2.28 Measurement of macroscopic variables

2 OBJECTS

2.1 Bulk systems

2.1.1 Gases
2.1.2 Supersonic beams
2.1.3 Liquids neat
2.1.4 Liquid mixtures and solutions
2.1.5 Crystals
2.1.5.1 neat *
2.1.5.2 mixed *
2.1.6 Glasses
2.1.7 Liquid crystals
2.1.8 Polymers
2.1.9 Semiconductors *
2.1.10 Metals and alloys *
2.1.11 Thin films *
2.1.12 Surfaces
2.1.13 Low-dimensional materials
2.1.14 Dielectrics *
2.1.15 Plasmas
2.1.16 Biological systems *

2.2 Microscopic systems

2.2.1 Atoms
2.2.2 Molecules (neutral and ionic)
2.2.2.1 diatomic
2.2.2.2 small polyatomics
2.2.2.3 aromatics
2.2.2.4 other large *
2.2.2.5 polymeric and biological
2.2.3 Molecular aggregates
2.2.3.1 dimers
2.2.3.2 van der Waals molecules
2.2.3.3 clusters
2.2.3.4 complexes *
2.2.4 Free radicals (including hydronium and muonium)
2.2.5 Quasiparticles (including excitons)
2.2.6 Defects and impurities *
2.2.7 Ions and charge carriers

* Denotes subject not covered in this volume.

3 PHENOMENA

3.1 Molecular structure
3.2 Vibrations and rotations of molecules
3.3 Electronic structure and states
3.4 Electric and magnetic properties
3.5 Spin splittings
3.6 Optical activity
3.7 Molecular interactions
3.8 Spectral bandshapes and intensities
3.9 Coupling of electronic and nuclear motion
3.10 Energy transfer processes
3.11 Molecular photophysical processes
3.12 Intramolecular dynamics
3.12.1 radiationless transitions *
3.12.2 vibrational energy distribution (including vibrational dissociation)
3.13 Luminescence spectra, yields and lifetimes
3.14 Coherence loss processes *
3.15 Non-linear responses (including optical) *
3.16 Multiphoton phenomena
3.17 Reactions (including dissociation)
3.17.1 gas phase
3.17.2 condensed phase
3.17.3 photochemical
3.18 Tunnelling *
3.19 Electron transfer
3.20 Positron annihilation *
3.21 Ionization (including Rydberg states)
3.22 Molecular motion (including diffusive)
3.23 Isotopic effects *
3.24 Fluctuations and noise
3.25 Collective motion and excitations
3.26 Surface effects and catalysis
3.27 Thermodynamic and transport properties *
3.28 Structure of solids and liquids
3.29 Critical phenomena *
3.30 Phase transitions *

SUBJECT INDEX TO VOLUME 112

METHODS

Theoretical

Group theory and algebras
A new magneto-optical effect in Raman spectroscopy, D.L. Andrews 112 (1987) 61

Quantized field theory
A new magneto-optical effect in Raman spectroscopy, D.L. Andrews 112 (1987) 61

Many body and quasiparticle approaches
Dynamic coordinate separation and state-dependent potentials. An analysis of localization in helium, V. Mujica, Y. Li and O. Goscinski 112 (1987) 159
Structure and properties of non-classical polymers. IV. Magnetic properties of polymers with superexchange interaction, N.N. Tyutyulkov and S.H. Karabunarliev 112 (1987) 293

Coupling schemes and perturbative treatments
Perturbational and variational treatments of the Morse oscillator, I.L. Cooper 112 (1987) 67
Correlation and the charge distribution of atoms, J. Blomquist and H. Essén 112 (1987) 173
Effects of non-uniform electric fields on the convergence behavior of energy expansions, R. Larter and D.J. Malik 112 (1987) 301

Equilibrium statistical mechanics
Comparison of the rate constants for VV energy transfer in the gas and liquid phases, P.A. Madden and F. van Swol 112 (1987) 43

Statistical mechanics of stationary states
Sensitivity of chemical chiral systems to weak asymmetric factors, V.A. Avetisov, V.V. Kuz'min and S.A. Anikin 112 (1987) 179

Non-equilibrium thermodynamic and hydrodynamic theories
The Fokker–Planck–Langevin model for rotational brownian motion. IV. Asymmetric top molecules, D.H. Lee and R.E.D. McClung 112 (1987) 23
Comparison of the rate constants for VV energy transfer in the gas and liquid phases, P.A. Madden and F. van Swol 112 (1987) 43
Outer-sphere electron transfer reactions at an electrode, L.D. Zusman 112 (1987) 53
The general solution of the coagulation equation for branched polymers, T.A. Bak and B. Lu 112 (1987) 189
Age distributions in chemical kinetics, M.O. Vlad and V.T. Popa 112 (1987) 307

Ab initio schemes for stationary properties
Velocity-dependent property surfaces and the theory of vibrational circular dichroism, A.D. Buckingham, P.W. Fowler and P.A. Galwas 112 (1987) 1
Dynamic coordinate separation and state-dependent potentials. An analysis of localization in helium, V. Mujica, Y. Li and O. Goscinski 112 (1987) 159
Correlation and the charge distribution of atoms, J. Blomquist and H. Essén 112 (1987) 173
CI calculations of electron and X-ray scattering cross sections of non-linear molecules: H_2O and NH_3, M. Breitenstein, H. Meyer and A. Schweig 112 (1987) 199
Ab initio calculations of oxygen nuclear quadrupole coupling constants and oxygen and silicon NMR shielding constants in molecules containing Si–O bonds, J.A. Tossel and P. Lazzeretti 112 (1987) 205
^{14}N nuclear quadrupole coupling in solid cinnolin-4-ones. A study by nuclear quadrupole resonance, X-ray crystallography and ab initio calculations, M.H. Palmer, R.O. Gould, A.J. Blake, J.A.S. Smith, D. Stephenson and D.E. Ames 112 (1987) 213
Effects of non-uniform electric fields on the convergence behavior of energy expansions, R. Larter and D.J. Malik 112 (1987) 301
Non-orthonormal basis calculations of the dipole transition moment for the Phillips system ($A^1\Pi_u \rightarrow X^1\Sigma_g^+$) in C_2. Theoretical lifetime of the $A^1\Pi_u$ state, G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker 112 (1987) 319
Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. I. The design of a one-electron effective core potential which includes 3d relaxation effects, I. Panas, P. Siegbahn and U. Wahlgren 112 (1987) 325
Calculation of the valence shell correlation effects on ionization potentials. A test on N_2, C_2N_2 and H_2NN, P. Decleva and A. Lisini 112 (1987) 339
Spin-forbidden transitions in the presence of an intersystem crossing: application to the $b^1\Sigma^+$ state in OH^+, R. de Vivie, C.M. Marian and S.D. Peyerimhoff 112 (1987) 349
The hfi parameters and structure of radical-anions of substituted tetra- and pentafluorobenzenes. Theory and experiment (OD ESR), V.V. Lozovoy, V.M. Grigoryants, O.A. Anisimov, Yu.N. Molin, P.V. Schastnev, L.N. Shchegoleva, I.I. Bilkis and V.D. Shteingarts 112 (1987) 463

Computational and simulation methods
Test of a modified sudden approximation for rotational excitation in He + CH_3CN, D.C. Clary and S. Green 112 (1987) 15
Electrostatic solvation energy in electrolyte solutions: a self-consistent inhomogeneous continuum model, A. Raudino, F. Zuccarello and G. Buemi 112 (1987) 77
The effect of reagent rotation on reaction cross sections for $O(^3P) + HCl \rightarrow OH + Cl$: a rationale for contradictory predictions, H. Loesch 112 (1987) 85
Cross sections for rotational/vibrational transitions in HF–HF collisions: effect of initial state, G.D. Billing 112 (1987) 95
Theoretical studies of photoexcitation and ionization in hydrogen sulfide, G.H.F. Diercksen and P.W. Langhoff 112 (1987) 227

Molecular dynamics and scattering theory
Test of a modified sudden approximation for rotational excitation in He + CH_3CN, D.C. Clary and S. Green 112 (1987) 15
The effect of reagent rotation on reaction cross sections for $O(^3P) + HCl \rightarrow OH + Cl$: a rationale for contradictory predictions, H. Loesch 112 (1987) 85

Cross sections for rotational/vibrational transitions in HF–HF collisions: effect of initial state, G.D. Billing 112 (1987) 95
CI calculations of electron and X-ray scattering cross sections of non-linear molecules: H_2O and NH_3, M. Breitenstein, H. Meyer and A. Schweig 112 (1987) 199
Possibility of detecting oscillations in near resonance Raman scattering, A. Lőrincz 112 (1987) 245
Vibrational analysis of $N_2(B\,^3\Pi_g$ and $C\,^3\Pi_u)$ and CO(X) excited in N_2 discharge and post discharge, S. de Benedictis and F. Cramarossa 112 (1987) 363

Experimental

Magnetic resonances

^{14}N nuclear quadrupole coupling in solid cinnolin-4-ones. A study by nuclear quadrupole resonance, X-ray crystallography and ab initio calculations, M.H. Palmer, R.O. Gould, A.J. Blake, J.A.S. Smith, D. Stephenson and D.E. Ames 112 (1987) 213
Zero-field NMR and NQR line shapes in the presence of brownian rotational reorientations, Yu.A. Serebrennikov 112 (1987) 253
The field dependence of CIDNP in gas-phase reactions of biradicals, A.V. Yurkovskaya, R.R. Galimov, A.A. Obynochny, K.M. Salikhov and R.Z. Sagdeev 112 (1987) 259
Linear dichroism of molecules with cubic symmetry, L.B.-Å. Johansson, G. Wikander, G. Lindblom and Å. Davidsson 112 (1987) 373
The hfi parameters and structure of radical-anions of substituted tetra- and pentafluorobenzenes. Theory and experiment (OD ESR), V.V. Lozovoy, V.M. Grigoryants, O.A. Anisimov, Yu.N. Molin, P.V. Schastnev, L.N. Shchegoleva, I.I. Bilkis and V.D. Shteingarts 112 (1987) 463

Infrared spectroscopy

Vibrational analysis of $N_2(B\,^3\Pi_g$ and $C\,^3\Pi_u)$ and CO(X) excited in N_2 discharge and post discharge, S. de Benedictis and F. Cramarossa 112 (1987) 363
Infrared spectroscopic studies of hydrogen-bonded complexes in cryogenic solutions, T.A. Iskanderov, Ya.M. Kimel'fel'd and E.M. Smirnova 112 (1987) 379
IR matrix spectra of $CsNO_2$, $RbNO_2$, KNO_2 and $NaNO_2$. The structure of $CsNO_2$, M. Barbeschi, L. Bencivenni and F. Ramondo 112 (1987) 387

Raman spectroscopy

Fabry–Perot spectra of depolarized Rayleigh wing in water: a new analysis of its temperature dependence, V. Mazzacurati and P. Benassi 112 (1987) 147

Visible and UV spectroscopy

Internal energy disposal in the chemiluminescent reaction CD + NO → ND(A) + CO and the kinetic isotope effect, N. Nishiyama, H. Sekiya, M. Tsuji and Y. Nishimura 112 (1987) 265
Magnetically perturbed, temperature-dependent and time-resolved aspects of the polarized luminescence of $Ru(bpy)_3^{2+}$ below 10 K, J. Ferguson and E. Krausz 112 (1987) 271
Vibrational analysis of $N_2(B\,^3\Pi_g$ and $C\,^3\Pi_u)$ and CO(X) excited in N_2 discharge and post discharge, S. de Benedictis and F. Cramarossa 112 (1987) 363
Linear dichroism of molecules with cubic symmetry, L.B.-Å. Johansson, G. Wikander, G. Lindblom and Å. Davidsson 112 (1987) 373

Fluorescence spectroscopy
Internal energy disposal in the chemiluminescent reaction CD + NO → ND(A) + CO and the kinetic isotope effect, N. Nishiyama, H. Sekiya, M. Tsuji and Y. Nishimura 112 (1987) 265
Magnetically perturbed, temperature-dependent and time-resolved aspects of the polarized luminescence of $Ru(bpy)_3^{2+}$ below 10 K, J. Ferguson and E. Krausz 112 (1987) 271
Site-selective fluorescence and hole-burning spectroscopy of MTHF glasses doped wih tetracene or pentacene, A. Elschner and H. Bässler 112 (1987) 285
Effect of guest–host interaction on spectra and relaxation dynamics of matrix-isolated Br_2 $B\,^3\Pi_{0^+u}$, $A\,^3\Pi_{1u}$ and $A'\,^3\Pi_{2u}$, J. Langen, K.-P. Lodemann and U. Schurath 112 (1987) 393

Laser methods
IR laser-induced decomposition of volatile uranyl complexes. I. Analysis of molecular beam depletions, M.R. Levy, D.M. Cox and A. Kaldor 112 (1987) 105
IR laser-induced decomposition of volatile uranyl complexes. II. New double resonance results, M.R. Levy, R.O. Brickman and A. Kaldor 112 (1987) 123
Electric dipole moments of the MgO $B\,^1\Sigma^+$ and $X\,^1\Sigma^+$ states, H. Büsener, F. Heinrich and A. Hese 112 (1987) 139
Kinetics of $CH(X\,^2\Pi)$ radical reactions with propane, isobutane and neopentane, S. Zabarnick, J.W. Fleming and M.C. Lin 112 (1987) 409

Multiple resonance spectroscopy
^{14}N nuclear quadrupole coupling in solid cinnolin-4-ones. A study by nuclear quadrupole resonance, X-ray crystallography and ab initio calculations, M.H. Palmer, R.O. Gould, A.J. Blake, J.A.S. Smith, D. Stephenson and D.E. Ames 112 (1987) 213

Atomic and molecular beam techniques
IR laser-induced decomposition of volatile uranyl complexes. I. Analysis of molecular beam depletions, M.R. Levy, D.M. Cox and A. Kaldor 112 (1987) 105
Charge-transfer collisions of potassium and rubidium with chlorine clusters: collision-energy dependence of cluster-products, U. Ross and T. Schulze 112 (1987) 415
Jet spectroscopy of pyrene complexes: unusual complexation shifts in the $S_0 \rightarrow S_1$ spectrum, E.A. Mangle and M.R. Topp 112 (1987) 427
The effect of molecular symmetry in alkane complexes of 2,5-diphenylfuran and related species, E.A. Mangle, A.L. Motyka, P. Salvi and M.R. Topp 112 (1987) 443

Time-resolved experiments
Electric dipole moments of the MgO $B\,^1\Sigma^+$ and $X\,^1\Sigma^+$ states, H. Büsener, F. Heinrich and A. Hese 112 (1987) 139
Magnetically perturbed, temperature-dependent and time-resolved aspects of the polarized luminescence of $Ru(bpy)_3^{2+}$ below 10 K, J. Ferguson and E. Krausz 112 (1987) 271
Effect of guest–host interaction on spectra and relaxation dynamics of matrix-isolated Br_2 $B\,^3\Pi_{0^+u}$, $A\,^3\Pi_{1u}$ and $A'\,^3\Pi_{2u}$, J. Langen, K.-P. Lodemann and U. Schurath 112 (1987) 393
Kinetics of $CH(X\,^2\Pi)$ radical reactions with propane, isobutane and neopentane, S. Zabarnick, J.W. Fleming and M.C. Lin 112 (1987) 409
Recombination of charge carriers in anthracene, P. Petelenz, V.H. Smith Jr., J. Klein, P. Martin and R. Voltz 112 (1987) 457

X-ray, electron and neutron diffraction
^{14}N nuclear quadrupole coupling in solid cinnolin-4-ones. A study by nuclear quadrupole resonance, X-ray crystallography and ab initio calculations, M.H. Palmer, R.O. Gould, A.J. Blake, J.A.S. Smith, D. Stephenson and D.E. Ames 112 (1987) 213

Light scattering
Fabry–Perot spectra of depolarized Rayleigh wing in water: a new analysis of its temperature dependence, V. Mazzacurati and P. Benassi 112 (1987) 147

Measurement of macroscopic variables
Linear dichroism of molecules with cubic symmetry, L.B.-Å. Johansson, G. Wikander, G. Lindblom and Å. Davidsson 112 (1987) 373

OBJECTS

Bulk systems

Gases
Cross sections for rotational/vibrational transitions in HF–HF collisions: effect of initial state, G.D. Billing 112 (1987) 95
The field dependence of CIDNP in gas-phase reactions of biradicals, A.V. Yurkovskaya, R.R. Galimov, A.A. Obynochny, K.M. Salikhov and R.Z. Sagdeev 112 (1987) 259
Age distributions in chemical kinetics, M.O. Vlad and V.T. Popa 112 (1987) 307

Supersonic beams
Jet spectroscopy of pyrene complexes: unusual complexation shifts in the $S_0 \rightarrow S_1$ spectrum, E.A. Mangle and M.R. Topp 112 (1987) 427
The effect of molecular symmetry in alkane complexes of 2,5-diphenylfuran and related species, E.A. Mangle, A.L. Motyka, P. Salvi and M.R. Topp 112 (1987) 443

Liquids neat
Fabry–Perot spectra of depolarized Rayleigh wing in water: a new analysis of its temperature dependence, V. Mazzacurati and P. Benassi 112 (1987) 147

Liquid mixtures and solutions
Comparison of the rate constants for VV energy transfer in the gas and liquid phases, P.A. Madden and F. van Swol 112 (1987) 43
Electrostatic solvation energy in electrolyte solutions: a self-consistent inhomogeneous continuum model, A. Raudino, F. Zuccarello and G. Buemi 112 (1987) 77
Infrared spectroscopic studies of hydrogen-bonded complexes in cryogenic solutions, T.A. Iskanderov, Ya.M. Kimel'fel'd and E.M. Smirnova 112 (1987) 379

Crystals
Magnetically perturbed, temperature-dependent and time-resolved aspects of the polarized luminescence of $Ru(bpy)_3^{2+}$ below 10 K, J. Ferguson and E. Krausz 112 (1987) 271

Glasses
Site-selective fluorescence and hole-burning spectroscopy of MTHF glasses doped wih tetracene or pentacene, A. Elschner and H. Bässler 112 (1987) 285

Liquid crystals
Linear dichroism of molecules with cubic symmetry, L.B.-Å. Johansson, G. Wikander, G. Lindblom and Å. Davidsson 112 (1987) 373

Polymers
The general solution of the coagulation equation for branched polymers, T.A. Bak and B. Lu 112 (1987) 189
Structure and properties of non-classical polymers. IV. Magnetic properties of polymers with superexchange interaction, N.N. Tyutyulkov and S.H. Karabunarliev 112 (1987) 293

Surfaces
Outer-sphere electron transfer reactions at an electrode, L.D. Zusman 112 (1987) 53
Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. I. The design of a one-electron effective core potential which includes 3d relaxation effects, I. Panas, P. Siegbahn and U. Wahlgren 112 (1987) 325

Low-dimensional materials
Structure and properties of non-classical polymers. IV. Magnetic properties of polymers with superexchange interaction, N.N. Tyutyulkov and S.H. Karabunarliev 112 (1987) 293

Plasmas
Vibrational analysis of $N_2(B\,^3\Pi_g$ and $C\,^3\Pi_u)$ and CO(X) excited in N_2 discharge and post discharge, S. de Benedictis and F. Cramarossa 112 (1987) 363

Microscopic systems

Atoms
Dynamic coordinate separation and state-dependent potentials. An analysis of localization in helium, V. Mujica, Y. Li and O. Goscinski 112 (1987) 159
Correlation and the charge distribution of atoms, J. Blomquist and H. Essén 112 (1987) 173

Molecules (neutral and ionic)
Velocity-dependent property surfaces and the theory of vibrational circular dichroism, A.D. Buckingham, P.W. Fowler and P.A. Galwas 112 (1987) 1
Sensitivity of chemical chiral systems to weak asymmetric factors, V.A. Avetisov, V.V. Kuz'min and S.A. Anikin 112 (1987) 179
Calculation of the valence shell correlation effects on ionization potentials. A test on N_2, C_2N_2 and H_2NN, P. Decleva and A. Lisini 112 (1987) 339
Vibrational analysis of $N_2(B\,^3\Pi_g$ and $C\,^3\Pi_u)$ and CO(X) excited in N_2 discharge and post discharge, S. de Benedictis and F. Cramarossa 112 (1987) 363
IR matrix spectra of $CsNO_2$, $RbNO_2$, KNO_2 and $NaNO_2$. The structure of $CsNO_2$, M. Barbeschi, L. Bencivenni and F. Ramondo 112 (1987) 387

– *diatomic*
Comparison of the rate constants for VV energy transfer in the gas and liquid phases, P.A. Madden and F. van Swol 112 (1987) 43
Perturbational and variational treatments of the Morse oscillator, I.L. Cooper 112 (1987) 67
Cross sections for rotational/vibrational transitions in HF–HF collisions: effect of initial state, G.D. Billing 112 (1987) 95
Electric dipole moments of the MgO $B^1\Sigma^+$ and $X^1\Sigma^+$ states, H. Büsener, F. Heinrich and A. Hese 112 (1987) 139
Effects of non-uniform electric fields on the convergence behavior of energy expansions, R. Larter and D.J. Malik 112 (1987) 301
Non-orthonormal basis calculations of the dipole transition moment for the Phillips system ($A^1\Pi_u \rightarrow X^1\Sigma_g^+$) in C_2. Theoretical lifetime of the $A^1\Pi_u$ state, G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker 112 (1987) 319
Spin-forbidden transitions in the presence of an intersystem crossing: application to the $b|^1\Sigma^+$ state in OH^+, R. de Vivie, C.M. Marian and S.D. Peyerimhoff 112 (1987) 349
Effect of guest–host interaction on spectra and relaxation dynamics of matrix-isolated Br_2 $B\,^3\Pi_{0^+}u$, $A^3\Pi_{1u}$ and $A'\,^3\Pi_{2u}$, J. Langen, K.-P. Lodemann and U. Schurath 112 (1987) 393

– *small polyatomics*
CI calculations of electron and X-ray scattering cross sections of non-linear molecules: H_2O and NH_3, M. Breitenstein, H. Meyer and A. Schweig 112 (1987) 199
Ab initio calculations of oxygen nuclear quadrupole coupling constants and oxygen and silicon NMR shielding constants in molecules containing Si–O bonds, J.A. Tossel and P. Lazzeretti 112 (1987) 205
Theoretical studies of photoexcitation and ionization in hydrogen sulfide, G.H.F. Diercksen and P.W. Langhoff 112 (1987) 227
IR matrix spectra of $CsNO_2$, $RbNO_2$, KNO_2 and $NaNO_2$. The structure of $CsNO_2$, M. Barbeschi, L. Bencivenni and F. Ramondo 112 (1987) 387

– *aromatics*
The hfi parameters and structure of radical-anions of substituted tetra- and pentafluorobenzenes. Theory and experiment (OD ESR), V.V. Lozovoy, V.M. Grigoryants, O.A. Anisimov, Yu.N. Molin, P.V. Schastnev, L.N. Shchegoleva, I.I. Bilkis and V.D. Shteingarts 112 (1987) 463

– *polymeric and biological*
The general solution of the coagulation equation for branched polymers, T.A. Bak and B. Lu 112 (1987) 189

Molecular aggregates
Infrared spectroscopic studies of hydrogen-bonded complexes in cryogenic solutions, T.A. Iskanderov, Ya.M. Kimel'fel'd and E.M. Smirnova 112 (1987) 379

– *dimers*
Infrared spectroscopic studies of hydrogen-bonded complexes in cryogenic solutions, T.A. Iskanderov, Ya.M. Kimel'fel'd and E.M. Smirnova 112 (1987) 379
Charge-transfer collisions of potassium and rubidium with chlorine clusters: collision-energy dependence of cluster-products, U. Ross and T. Schulze 112 (1987) 415

– van der Waals molecules
Test of a modified sudden approximation for rotational excitation in He + CH_3CN, D.C. Clary and S. Green 112 (1987) 15
Jet spectroscopy of pyrene complexes: unusual complexation shifts in the $S_0 \rightarrow S_1$ spectrum, E.A. Mangle and M.R. Topp 112 (1987) 427
The effect of molecular symmetry in alkane complexes of 2,5-diphenylfuran and related species, E.A. Mangle, A.L. Motyka, P. Salvi and M.R. Topp 112 (1987) 443

– clusters
The general solution of the coagulation equation for branched polymers, T.A. Bak and B. Lu 112 (1987) 189
Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. I. The design of a one-electron effective core potential which includes 3d relaxation effects, I. Panas, P. Siegbahn and U. Wahlgren 112 (1987) 325
Charge-transfer collisions of potassium and rubidium with chlorine clusters: collision-energy dependence of cluster-products, U. Ross and T. Schulze 112 (1987) 415

Free radicals (including hydronium and muonium)
The field dependence of CIDNP in gas-phase reactions of biradicals, A.V. Yurkovskaya, R.R. Galimov, A.A. Obynochny, K.M. Salikhov and R.Z. Sagdeev 112 (1987) 259
Kinetics of $CH(X\,^2\Pi)$ radical reactions with propane, isobutane and neopentane, S. Zabarnick, J.W. Fleming and M.C. Lin 112 (1987) 409

Quasiparticles (including excitons)
Recombination of charge carriers in anthracene, P. Petelenz, V.H. Smith Jr., J. Klein, P. Martin and R. Voltz 112 (1987) 457

Ions and charge carriers
Outer-sphere electron transfer reactions at an electrode, L.D. Zusman 112 (1987) 53
Recombination of charge carriers in anthracene, P. Petelenz, V.H. Smith Jr., J. Klein, P. Martin and R. Voltz 112 (1987) 457

PHENOMENA

Molecular structure
Sensitivity of chemical chiral systems to weak asymmetric factors, V.A. Avetisov, V.V. Kuz'min and S.A. Anikin 112 (1987) 179
Non-orthonormal basis calculations of the dipole transition moment for the Phillips system ($A^1\Pi_u \rightarrow X\,^1\Sigma_g^+$) in C_2. Theoretical lifetime of the $A^1\Pi_u$ state, G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker 112 (1987) 319
Spin-forbidden transitions in the presence of an intersystem crossing: application to the $b^1\Sigma^+$ state in OH^+, R. de Vivie, C.M. Marian and S.D. Peyerimhoff 112 (1987) 349
IR matrix spectra of $CsNO_2$, $RbNO_2$, KNO_2 and $NaNO_2$. The structure of $CsNO_2$, M. Barbeschi, L. Bencivenni and F. Ramondo 112 (1987) 387
The hfi parameters and structure of radical-anions of substituted tetra- and pentafluorobenzenes. Theory and experiment (OD ESR), V.V. Lozovoy, V.M. Grigoryants, O.A. Anisimov, Yu.N. Molin, P.V. Schastnev, L.N. Shchegoleva, I.I. Bilkis and V.D. Shteingarts 112 (1987) 463

Vibrations and rotations of molecules
A new magneto-optical effect in Raman spectroscopy, D.L. Andrews 112 (1987) 61
Perturbational and variational treatments of the Morse oscillator, I.L. Cooper 112 (1987) 67
Internal energy disposal in the chemiluminescent reaction CD + NO → ND(A) + CO and the kinetic isotope effect, N. Nishiyama, H. Sekiya, M. Tsuji and Y. Nishimura 112 (1987) 265

Electronic structure and states
Dynamic coordinate separation and state-dependent potentials. An analysis of localization in helium, V. Mujica, Y. Li and O. Goscinski 112 (1987) 159
Correlation and the charge distribution of atoms, J. Blomquist and H. Essén 112 (1987) 173
CI calculations of electron and X-ray scattering cross sections of non-linear molecules: H_2O and NH_3, M. Breitenstein, H. Meyer and A. Schweig 112 (1987) 199
Theoretical studies of photoexcitation and ionization in hydrogen sulfide, G.H.F. Diercksen and P.W. Langhoff 112 (1987) 227
Effects of non-uniform electric fields on the convergence behavior of energy expansions, R. Larter and D.J. Malik 112 (1987) 301
Calculation of the valence shell correlation effects on ionization potentials. A test on N_2, C_2N_2 and H_2NN, P. Decleva and A. Lisini 112 (1987) 339
Linear dichroism of molecules with cubic symmetry, L.B.-Å. Johansson, G. Wikander, G. Lindblom and Å. Davidsson 112 (1987) 373

Electric and magnetic properties
Velocity-dependent property surfaces and the theory of vibrational circular dichroism, A.D. Buckingham, P.W. Fowler and P.A. Galwas 112 (1987) 1
A new magneto-optical effect in Raman spectroscopy, D.L. Andrews 112 (1987) 61
Electric dipole moments of the MgO $B^1\Sigma^+$ and $X^1\Sigma^+$ states, H. Büsener, F. Heinrich and A. Hese 112 (1987) 139
Ab initio calculations of oxygen nuclear quadrupole coupling constants and oxygen and silicon NMR shielding constants in molecules containing Si–O bonds, J.A. Tossel and P. Lazzeretti 112 (1987) 205
Structure and properties of non-classical polymers. IV. Magnetic properties of polymers with superexchange interaction, N.N. Tyutyulkov and S.H. Karabunarliev 112 (1987) 293
Effects of non-uniform electric fields on the convergence behavior of energy expansions, R. Larter and D.J. Malik 112 (1987) 301

Spin splittings
The hfi parameters and structure of radical-anions of substituted tetra- and pentafluorobenzenes. Theory and experiment (OD ESR), V.V. Lozovoy, V.M. Grigoryants, O.A. Anisimov, Yu.N. Molin, P.V. Schastnev, L.N. Shchegoleva, I.I. Bilkis and V.D. Shteingarts 112 (1987) 463

Optical activity
Velocity-dependent property surfaces and the theory of vibrational circular dichroism, A.D. Buckingham, P.W. Fowler and P.A. Galwas 112 (1987) 1

Molecular interactions
Test of a modified sudden approximation for rotational excitation in He + CH_3CN, D.C. Clary and S. Green 112 (1987) 15

Electrostatic solvation energy in electrolyte solutions: a self-consistent inhomogeneous continuum model, A. Raudino, F. Zuccarello and G. Buemi 112 (1987) 77
Infrared spectroscopic studies of hydrogen-bonded complexes in cryogenic solutions, T.A. Iskanderov, Ya.M. Kimel'fel'd and E.M. Smirnova 112 (1987) 379
Jet spectroscopy of pyrene complexes: unusual complexation shifts in the $S_0 \rightarrow S_1$ spectrum, E.A. Mangle and M.R. Topp 112 (1987) 427
The effect of molecular symmetry in alkane complexes of 2,5-diphenylfuran and related species, E.A. Mangle, A.L. Motyka, P. Salvi and M.R. Topp 112 (1987) 443

Spectral bandshapes and intensities
The Fokker–Planck–Langevin model for rotational brownian motion. IV. Asymmetric top molecules, D.H. Lee and R.E.D. McClung 112 (1987) 23
A new magneto-optical effect in Raman spectroscopy, D.L. Andrews 112 (1987) 61
Zero-field NMR and NQR line shapes in the presence of brownian rotational reorientations, Yu.A. Serebrennikov 112 (1987) 253
Non-orthonormal basis calculations of the dipole transition moment for the Phillips system ($A^1\Pi_u \rightarrow X^1\Sigma_g^+$) in C_2. Theoretical lifetime of the $A^1\Pi_u$ state, G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker 112 (1987) 319

Coupling of electronic and nuclear motion
Velocity-dependent property surfaces and the theory of vibrational circular dichroism, A.D. Buckingham, P.W. Fowler and P.A. Galwas 112 (1987) 1
Dynamic coordinate separation and state-dependent potentials. An analysis of localization in helium, V. Mujica, Y. Li and O. Goscinski 112 (1987) 159
Spin-forbidden transitions in the presence of an intersystem crossing: application to the $b^1\Sigma^+$ state in OH^+, R. de Vivie, C.M. Marian and S.D. Peyerimhoff 112 (1987) 349

Energy transfer processes
Test of a modified sudden approximation for rotational excitation in He + CH_3CN, D.C. Clary and S. Green 112 (1987) 15
Comparison of the rate constants for VV energy transfer in the gas and liquid phases, P.A. Madden and F. van Swol 112 (1987) 43
Cross sections for rotational/vibrational transitions in HF–HF collisions: effect of initial state, G.D. Billing 112 (1987) 95
Vibrational analysis of $N_2(B\,^3\Pi_g$ and $C\,^3\Pi_u)$ and CO(X) excited in N_2 discharge and post discharge, S. de Benedictis and F. Cramarossa 112 (1987) 363
Charge-transfer collisions of potassium and rubidium with chlorine clusters: collision-energy dependence of cluster-products, U. Ross and T. Schulze 112 (1987) 415

Molecular photophysical processes
Theoretical studies of photoexcitation and ionization in hydrogen sulfide, G.H.F. Diercksen and P.W. Langhoff 112 (1987) 227
Possibility of detecting oscillations in near resonance Raman scattering, A. Lőrincz 112 (1987) 245
Site-selective fluorescence and hole-burning spectroscopy of MTHF glasses doped wih tetracene or pentacene, A. Elschner and H. Bässler 112 (1987) 285
Non-orthonormal basis calculations of the dipole transition moment for the Phillips system ($A^1\Pi_u \rightarrow X^1\Sigma_g^+$) in C_2. Theoretical lifetime of the $A^1\Pi_u$ state, G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker 112 (1987) 319

Effect of guest–host interaction on spectra and relaxation dynamics of matrix-isolated Br_2 $B\,^3\Pi_{0^+}u$, $A^3\Pi_{1u}$ and $A'\,^3\Pi_{2u}$, J. Langen, K.-P. Lodemann and U. Schurath 112 (1987) 393

Intramolecular dynamics
Spin-forbidden transitions in the presence of an intersystem crossing: application to the $b^1\Sigma^+$ state in OH^+, R. de Vivie, C.M. Marian and S.D. Peyerimhoff 112 (1987) 349

– vibrational energy redistribution (including vibrational dissociation)
IR laser-induced decomposition of volatile uranyl complexes. I. Analysis of molecular beam depletions, M.R. Levy, D.M. Cox and A. Kaldor 112 (1987) 105
IR laser-induced decomposition of volatile uranyl complexes. II. New double resonance results, M.R. Levy, R.O. Brickman and A. Kaldor 112 (1987) 123
Internal energy disposal in the chemiluminescent reaction CD + NO → ND(A) + CO and the kinetic isotope effect, N. Nishiyama, H. Sekiya, M. Tsuji and Y. Nishimura 112 (1987) 265

Luminescence spectra, yields and lifetimes
Magnetically perturbed, temperature-dependent and time-resolved aspects of the polarized luminescence of $Ru(bpy)_3^{2+}$ below 10 K, J. Ferguson and E. Krausz 112 (1987) 271
Site-selective fluorescence and hole-burning spectroscopy of MTHF glasses doped wih tetracene or pentacene, A. Elschner and H. Bässler 112 (1987) 285
Effect of guest–host interaction on spectra and relaxation dynamics of matrix-isolated Br_2 $B\,^3\Pi_{0^+}u$, $A^3\Pi_{1u}$ and $A'\,^3\Pi_{2u}$, J. Langen, K.-P. Lodemann and U. Schurath 112 (1987) 393
Recombination of charge carriers in anthracene, P. Petelenz, V.H. Smith Jr., J. Klein, P. Martin and R. Voltz 112 (1987) 457

Multiphoton phenomena
IR laser-induced decomposition of volatile uranyl complexes. I. Analysis of molecular beam depletions, M.R. Levy, D.M. Cox and A. Kaldor 112 (1987) 105
IR laser-induced decomposition of volatile uranyl complexes. II. New double resonance results, M.R. Levy, R.O. Brickman and A. Kaldor 112 (1987) 123

Reactions (including dissociation)
The effect of reagent rotation on reaction cross sections for $O(^3P) + HCl \rightarrow OH + Cl$: a rationale for contradictory predictions, H. Loesch 112 (1987) 85
Age distributions in chemical kinetics, M.O. Vlad and V.T. Popa 112 (1987) 307

– gas phase
The effect of reagent rotation on reaction cross sections for $O(^3P) + HCl \rightarrow OH + Cl$: a rationale for contradictory predictions, H. Loesch 112 (1987) 85
IR laser-induced decomposition of volatile uranyl complexes. I. Analysis of molecular beam depletions, M.R. Levy, D.M. Cox and A. Kaldor 112 (1987) 105
IR laser-induced decomposition of volatile uranyl complexes. II. New double resonance results, M.R. Levy, R.O. Brickman and A. Kaldor 112 (1987) 123
The field dependence of CIDNP in gas-phase reactions of biradicals, A.V. Yurkovskaya, R.R. Galimov, A.A. Obynochny, K.M. Salikhov and R.Z. Sagdeev 112 (1987) 259
Internal energy disposal in the chemiluminescent reaction CD + NO → ND(A) + CO and the kinetic isotope effect, N. Nishiyama, H. Sekiya, M. Tsuji and Y. Nishimura 112 (1987) 265

Kinetics of CH($X\,^2\Pi$) radical reactions with propane, isobutane and neopentane, S. Zabarnick, J.W. Fleming and M.C. Lin 112 (1987) 409

– condensed phase
The general solution of the coagulation equation for branched polymers, T.A. Bak and B. Lu 112 (1987) 189
Charge-transfer collisions of potassium and rubidium with chlorine clusters: collision-energy dependence of cluster-products, U. Ross and T. Schulze 112 (1987) 415

– photochemical
The field dependence of CIDNP in gas-phase reactions of biradicals, A.V. Yurkovskaya, R.R. Galimov, A.A. Obynochny, K.M. Salikhov and R.Z. Sagdeev 112 (1987) 259

Electron transfer
Outer-sphere electron transfer reactions at an electrode, L.D. Zusman 112 (1987) 53
Recombination of charge carriers in anthracene, P. Petelenz, V.H. Smith Jr., J. Klein, P. Martin and R. Voltz 112 (1987) 457

Ionization (including Rydberg states)
Theoretical studies of photoexcitation and ionization in hydrogen sulfide, G.H.F. Diercksen and P.W. Langhoff 112 (1987) 227
Calculation of the valence shell correlation effects on ionization potentials. A test on N_2, C_2N_2 and H_2NN, P. Decleva and A. Lisini 112 (1987) 339

Molecular motion (including diffusive)
The Fokker–Planck–Langevin model for rotational brownian motion. IV. Asymmetric top molecules, D.H. Lee and R.E.D. McClung 112 (1987) 23
Zero-field NMR and NQR line shapes in the presence of brownian rotational reorientations, Yu.A. Serebrennikov 112 (1987) 253

Fluctuations and noise
Outer-sphere electron transfer reactions at an electrode, L.D. Zusman 112 (1987) 53
Age distributions in chemical kinetics, M.O. Vlad and V.T. Popa 112 (1987) 307

Collective motion and excitations
Fabry–Perot spectra of depolarized Rayleigh wing in water: a new analysis of its temperature dependence, V. Mazzacurati and P. Benassi 112 (1987) 147

Surface effects and catalysis
Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. I. The design of a one-electron effective core potential which includes 3d relaxation effects, I. Panas, P. Siegbahn and U. Wahlgren 112 (1987) 325

Structure of solids and liquids
Electrostatic solvation energy in electrolyte solutions: a self-consistent inhomogeneous continuum model, A. Raudino, F. Zuccarello and G. Buemi 112 (1987) 77